

# Renormalized parameters and perturbation theory for an $n$ -channel Anderson model with Hund's rule coupling.

Y Nishikawa<sup>1,2</sup> D J G Crow<sup>1</sup> and A C Hewson<sup>1</sup>

<sup>1</sup>*Department of Mathematics, Imperial College, London SW7 2AZ, UK. and*

<sup>2</sup>*Graduate School of Science, Osaka City University, Osaka 558-8585, Japan*

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We extend the renormalized perturbation theory for the single impurity Anderson model to the  $n$ -channel model with a Hund's rule coupling, and show that the exact results for the spin, orbital and charge susceptibilities, as well as the leading low temperature dependence for the resistivity, are obtained by working to second order in the renormalized couplings. A universal relation is obtained between the renormalized parameters, independent of  $n$ , in the Kondo regime. An expression for the dynamic spin susceptibility is also derived by taking into account repeated quasiparticle scattering, which is asymptotically exact in the low frequency regime and satisfies the Korringa-Shiba relation. The renormalized parameters, including the renormalized Hund's rule coupling, are deduced from numerical renormalization group calculations for the model for the case  $n = 2$ . The results confirm explicitly the universal relations between the parameters in the Kondo regime. Using these results we evaluate the spin, orbital and charge susceptibilities, temperature dependence of the low temperature resistivity and dynamic spin susceptibility for the particle-hole symmetric  $n = 2$  model.

## I. INTRODUCTION

The single impurity Anderson model<sup>1</sup> has played an important role in understanding many aspects of the behavior of electrons in systems with strong electron correlation. Non-perturbative methods have had to be developed to make predictions for the behavior of the model in the strong interaction regime. Among the most successful have been the seminal and pioneering work of Wilson and associates<sup>2,3</sup> based on the numerical renormalization group (NRG), and the exact solutions using the Bethe ansatz for the linear dispersion version of the model<sup>4,5</sup>. Though the model was originally put forward to describe magnetic impurities in a host metal, it has proved to be applicable to other situations. One main area of application is as a model for strong correlation effects in quantum dots<sup>6</sup>. In this application certain parameters of the model, such as the impurity level which determines the electron occupancy on the quantum dot, can be varied by a gate voltage. This makes it possible to sweep through different parameter regimes of the model, which would be difficult to do for real magnetic impurities, and so the predictions of the model can be tested more rigorously. The presence of the narrow many-body resonance in the strong correlation (Kondo) regime at low temperatures can be inferred directly from the measurements of the current through the dot as a function of an applied bias voltage<sup>7,8</sup>.

Apart from these direct applications of the model, it has also played a role in the calculations of strong correlation effects in lattice models. It is possible to map a class of infinite dimensional lattice models of strong electron correlation onto an effective Anderson impurity model with a self-consistency condition, which determines the density of states of the effective medium<sup>9</sup>. This mapping requires that the self-energy is a function of frequency only which is the case in the limit of infinite dimensionality, and the mapping is exact in this limit. For many

strongly correlated systems it is known that the wave vector dependence of the self-energy is much less important than the frequency dependence so this approach can be used as a good first approximation for systems in three dimensions (dynamical mean field theory (DMFT)). As the assumption of linear dispersion is not valid for the effective impurity model generated in this application, there are no exact Bethe ansatz solutions, so the most reliable non-perturbative approaches, such as the NRG have to be used.

It has not proved possible so far to access the strong correlation regime of the Anderson model by an approach based purely on perturbation theory in powers of the local interaction  $U$ . However, it has been shown that, if the perturbation theory is reorganized such that the basic parameters of the model are renormalized, then a perturbation theory in the renormalized interaction  $\tilde{U}$ , taken only to second order gives formally the exact results for the low temperature properties and low frequency dynamics, provided counter terms are taken into account to avoid over-counting<sup>10,11</sup>. The renormalized parameters have to be determined but these can be calculated very accurately from an analysis of the low energy excitations of an NRG calculation on the approach to the low energy fixed point<sup>12</sup>. So far this approach has only been developed in detail for the non-degenerate one channel model, but the approach is one that can be applied to a more general class of models including lattice models. Here we extend the calculations to an  $n$ -channel impurity Anderson model with the inclusion of a Hund's rule exchange term. The Hamiltonian takes the form,

$$\mathcal{H} = \sum_{m\sigma} \epsilon_{dm\sigma} d_{m\sigma}^\dagger d_{m\sigma} + \sum_{k,m\sigma} \epsilon_{km\sigma} c_{km\sigma}^\dagger c_{km\sigma} + \sum_{km\sigma} (V_k d_{m\sigma}^\dagger c_{km\sigma} + V_k^* c_{km\sigma}^\dagger d_{m\sigma}) + \mathcal{H}_d \quad (1)$$

where  $d_{m\sigma}^\dagger$ ,  $d_{m\sigma}$ , are creation and annihilation opera-

tors for an electron in an impurity state with total angular momentum quantum number  $l$ , and  $z$ -component  $m = -l, -l+1, \dots, l$ , and spin component  $\sigma = \uparrow, \downarrow$ . The impurity level in a magnetic field  $H$  we take as  $\epsilon_{dm\sigma} = \epsilon_d - \mu_B \sigma H - \mu_B m H - \mu$ , where  $\sigma = 1$  ( $\uparrow$ ) and  $\sigma = -1$  ( $\downarrow$ ) and  $\mu$  is the chemical potential, and  $\mu_B$  the Bohr magneton. The creation and annihilation operators  $c_{km\sigma}^\dagger, c_{km\sigma}$  are for partial wave conduction electrons with energy  $\epsilon_{km\sigma}$ . The hybridization matrix element for impurity levels with the conduction electron states is  $V_k$ . We denote the hybridization width factor by  $\Delta_{m\sigma}(\epsilon) = \pi \sum_k |V_k|^2 \delta(\epsilon - \epsilon_{km\sigma})$ , which we can take to be a constant  $\Delta$  in the wide flat band limit. The remaining part of the Hamiltonian,  $\mathcal{H}_d$  describes the interaction between the electrons in the impurity state, which we take to be of the form,

$$\mathcal{H}_d = \frac{(U - J_H)}{2} \sum_{mm'\sigma\sigma'} d_{m\sigma}^\dagger d_{m'\sigma'}^\dagger d_{m'\sigma'} d_{m\sigma} + \frac{J_H}{2} \sum_{mm'\sigma\sigma'} d_{m\sigma}^\dagger d_{m'\sigma'}^\dagger d_{m\sigma} d_{m'\sigma'}. \quad (2)$$

As well as the direct Coulomb interaction  $U$  between the electrons, we include a Hund's rule exchange term  $J_H$  between electrons in states with different  $m$  values. The sign for the exchange term has been chosen so that  $J_H > 0$  corresponds to a ferromagnetic interaction. This model can be used to describe transition metal impurities, such as Mn or Fe, in a metallic host in the absence of spin orbit or crystal field splittings. We can interpret the model more generally with  $\alpha = m + l + 1$  as a channel index taking values  $\alpha = 1, 2, \dots, n$  where  $n$  is the number of channels. The Hund's rule term tends to align the electrons on the impurity site such that for large  $U$  and large  $J_H$  the impurity state will correspond to a spin  $S = n/2$ . The model with  $J_H = 0$  has also been used to describe capacitively coupled double quantum dots<sup>13</sup>, where the impurity channels correspond to different dots. In that application, however, the inter-dot interaction  $U'$  will in general differ from the intra-dot interaction  $U$ , so the case here, with  $U' = U$ , is a special point with  $SU(2n)$  symmetry when  $J_H = 0$ .

The structure of this paper will be as follows. In the next section we formulate the renormalized perturbation theory (RPT) for this model in terms of the renormalized parameters,  $\tilde{\epsilon}_d$ ,  $\tilde{\Delta}$ ,  $\tilde{U}$  and  $\tilde{J}_H$ . We then show that the low temperature behavior, as measured by the charge and spin susceptibilities and the low temperature contribution to the resistivity, can be obtained exactly from the RPT taken to second order in powers of  $\tilde{U}$  and  $\tilde{J}_H$ . In the localized or Kondo regime we show that  $\tilde{\Delta}$ ,  $\tilde{U}$  and  $\tilde{J}_H$  can be expressed in terms of a single parameter which we take as the Kondo temperature  $T_K$ . This relation is independent of the channel index  $n$  and hence applies to all values of  $n$ . Though we cannot calculate  $\tilde{\Delta}$ ,  $\tilde{U}$  and  $\tilde{J}_H$  for the general  $n$ -model using the NRG we can calculate them for the two channel case  $n = 2$ . We look at this case in detail and confirm the universal relation between the

renormalized parameters in the Kondo regime predicted using the RPT.

## II. RENORMALIZED PERTURBATION THEORY

We start with the Fourier transform of the single particle Green's function for the impurity  $d$ -state,

$$G_{d,\sigma}(\omega) = - \int_0^\beta \langle T_\tau d_{m\sigma}(\tau) d_{m\sigma}^\dagger(0) \rangle e^{i\omega_n \tau} d\tau, \quad (3)$$

where  $\omega_n = (2n' + 1)/\beta$  and  $\beta = 1/T$  and the brackets  $\langle \dots \rangle$  denote a thermal average.

$$G_{d,m\sigma}(\omega_n) = \frac{1}{i\omega_n - \epsilon_{dm\sigma} + i\Delta \text{sgn}(\omega_n) - \Sigma_{m\sigma}(\omega_n, H)}, \quad (4)$$

where  $\Sigma_{m\sigma}(\omega_n, H)$  is the self-energy. For the zero temperature Green's function, which will be our main concern,  $\omega_n$  can be replaced by continuous variable  $\omega$ , and summations over  $\omega_n$  replaced by integrations over  $\omega$ . For the perturbation theory in powers of  $U$  and  $J_H$  it will be convenient to separate the interaction terms in the Hamiltonian into the terms involving interactions between electrons in the same channel and those between electrons in different channels. We rewrite the Hamiltonian from Eq. (2) in the form,

$$\mathcal{H}_d = U \sum_m n_{d,m\uparrow} n_{d,m\downarrow} + \frac{(U - J_H)}{2} \sum_{m \neq m' \sigma \sigma'} d_{m\sigma}^\dagger d_{m'\sigma'}^\dagger d_{m'\sigma'} d_{m\sigma} + \frac{J_H}{2} \sum_{m \neq m' \sigma \sigma'} d_{m\sigma}^\dagger d_{m'\sigma'}^\dagger d_{m\sigma} d_{m'\sigma'}. \quad (5)$$

The vertices associated with the three types of interaction terms are illustrated in Fig. 1.

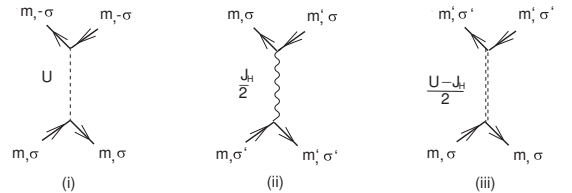


FIG. 1: (Color online) The three interaction vertices corresponding to the terms in the Hamiltonian given in Eq. (5).

For the renormalized perturbation theory, the Green's function in Eq. (4) can be re-expressed as  $G_{d,m\sigma}(\omega_n) =$

$z\tilde{G}_{d,m\sigma}(\omega_n)$ , where  $\tilde{G}_{d,m\sigma}(\omega_n)$  is the quasiparticle Green's function given by

$$\tilde{G}_{d,m\sigma}(\omega_n) = \frac{1}{i\omega_n - \tilde{\epsilon}_{dm\sigma} + i\tilde{\Delta}\text{sgn}(\omega_n) - \tilde{\Sigma}_{m\sigma}(\omega_n, H)} \quad (6)$$

and the renormalized parameters,  $\tilde{\epsilon}_{dm\sigma}$  and  $\tilde{\Delta}$  are given by

$$\tilde{\epsilon}_{dm\sigma} = z(\epsilon_d + \Sigma_{m\sigma}(0, H)) - \mu_B\sigma H - \mu_B m H, \quad \tilde{\Delta} = z\Delta, \quad (7)$$

where  $z = 1/(1 - \partial\Sigma_{m\sigma}(\omega, 0)/\partial(i\omega))$  evaluated at  $\omega = 0$ . The quasiparticle self-energy  $\tilde{\Sigma}_{m,\sigma}(\omega, H)$  is given by

$$\tilde{\Sigma}_{m\sigma}(\omega, H) = z \left( \Sigma_{m\sigma}(\omega, H) - \Sigma_{m\sigma}(0, H) - i\omega \frac{\partial\Sigma_{m\sigma}(\omega, 0)}{\partial i\omega} \Big|_{\omega=0} \right),$$

where we have assumed the Luttinger theorem<sup>14</sup>,  $\text{Im}\Sigma(0) = 0$ , so that  $\text{Im}\Sigma_{m\sigma}(\omega) \sim \omega^2$  as  $\omega \rightarrow 0$ . When expressed in this form, the  $\omega = 0$  part of the self-energy and its derivative have been absorbed into renormalizing the parameters  $\epsilon_{dm\sigma}$  and  $\Delta$ , so in setting up the perturbation expansion any further renormalization of these terms must be excluded, or it will result in overcounting. In working with the fully renormalized quasiparticles it is appropriate to use the renormalized or effective interactions between the quasiparticles. In the single channel case, we defined the renormalized interaction  $\tilde{U}$  in terms of the four vertex  $\Gamma_{\uparrow,\downarrow,\downarrow,\uparrow}(\omega_1, \omega_2, \omega_3, \omega_4)$  in the zero frequency limit<sup>10</sup>. In this case we need to consider the more general four vertex,  $\Gamma_{m_3\sigma_3; m_4\sigma_4}^{m_1\sigma_1; m_2\sigma_2}(\omega_1, \omega_2, \omega_3, \omega_4)$ , which corresponds to the Fourier coefficient of the connected skeleton diagram for the two particle Green's function,

$$\langle T_\tau d_{m_1\sigma_1}(\tau_1) d_{m_2\sigma_2}(\tau_2) d_{m_3\sigma_3}^\dagger(\tau_3) d_{m_4\sigma_4}^\dagger(\tau_4) \rangle, \quad (8)$$

with the external legs removed. Using the fact that the spin and angular momentum are conserved independently, and taking into account the antisymmetry conditions of the fermion creation and annihilation operators, it was shown by Yoshimori<sup>15</sup> that this vertex at zero frequency can be expressed in terms of two parameters,  $\Gamma_C$  and  $\Gamma_e$ , as

$$\begin{aligned} \Gamma_{m_3\sigma_3; m_4\sigma_4}^{m_1\sigma_1; m_2\sigma_2}(0, 0, 0, 0) = \\ \Gamma_C(\delta_{m_4}^{m_1} \delta_{m_3}^{m_2} \delta_{\sigma_4}^{\sigma_1} \delta_{\sigma_3}^{\sigma_2} - \delta_{m_3}^{m_1} \delta_{m_4}^{m_2} \delta_{\sigma_3}^{\sigma_1} \delta_{\sigma_4}^{\sigma_2}) \\ + \Gamma_e(\delta_{m_3}^{m_1} \delta_{m_4}^{m_2} \delta_{\sigma_4}^{\sigma_1} \delta_{\sigma_3}^{\sigma_2} - \delta_{m_4}^{m_1} \delta_{m_3}^{m_2} \delta_{\sigma_3}^{\sigma_1} \delta_{\sigma_4}^{\sigma_2}). \end{aligned} \quad (9)$$

To first order in the interaction terms,  $U$  and  $J_H$ , we have  $\Gamma_C = U - J_H$  and  $\Gamma_e = J_H$ . We generalize this result to specify the renormalized parameters,  $\tilde{U}$ , and  $\tilde{J}_H$ , by the relation,

$$\begin{aligned} z^2 \Gamma_{m_3\sigma_3; m_4\sigma_4}^{m_1\sigma_1; m_2\sigma_2}(0, 0, 0, 0) = \\ (\tilde{U} - \tilde{J}_H)(\delta_{m_4}^{m_1} \delta_{m_3}^{m_2} \delta_{\sigma_4}^{\sigma_1} \delta_{\sigma_3}^{\sigma_2} - \delta_{m_3}^{m_1} \delta_{m_4}^{m_2} \delta_{\sigma_3}^{\sigma_1} \delta_{\sigma_4}^{\sigma_2}) \\ + \tilde{J}_H(\delta_{m_3}^{m_1} \delta_{m_4}^{m_2} \delta_{\sigma_4}^{\sigma_1} \delta_{\sigma_3}^{\sigma_2} - \delta_{m_4}^{m_1} \delta_{m_3}^{m_2} \delta_{\sigma_3}^{\sigma_1} \delta_{\sigma_4}^{\sigma_2}), \end{aligned} \quad (10)$$

where the factor  $z^2$  arises from the rescaling of the fields to define the quasiparticle Green's function given in Eq. (6). For  $n = 1$  this reduces to

$$z^2 \Gamma_{\sigma_3; \sigma_4}^{\sigma_1; \sigma_2}(0, 0, 0, 0) = \tilde{U}(\delta_{\sigma_4}^{\sigma_1} \delta_{\sigma_3}^{\sigma_2} - \delta_{\sigma_3}^{\sigma_1} \delta_{\sigma_4}^{\sigma_2}), \quad (11)$$

which is the definition of  $\tilde{U}$  used in earlier work<sup>10</sup>.

We can combine these terms to define a quasiparticle Hamiltonian  $\tilde{H}$ ,

$$\begin{aligned} \tilde{H} = \sum_{m\sigma} \tilde{\epsilon}_{dm\sigma} \tilde{d}_{m\sigma}^\dagger \tilde{d}_{m\sigma} + \sum_{km\sigma} \epsilon_{km\sigma} c_{km\sigma}^\dagger c_{km\sigma} \\ + \sum_{km\sigma} (\tilde{V}_k \tilde{d}_{m\sigma}^\dagger c_{km\sigma} + \tilde{V}_k^* c_{km\sigma}^\dagger \tilde{d}_{m\sigma}) + \tilde{H}_d \end{aligned} \quad (12)$$

$$\begin{aligned} \tilde{H}_d = \frac{(\tilde{U} - \tilde{J}_H)}{2} \sum_{mm'\sigma\sigma'} : \tilde{d}_{m\sigma}^\dagger \tilde{d}_{m'\sigma'}^\dagger \tilde{d}_{m'\sigma'} \tilde{d}_{m\sigma} : \\ + \frac{\tilde{J}_H}{2} \sum_{mm'\sigma\sigma'} : \tilde{d}_{m\sigma}^\dagger \tilde{d}_{m'\sigma'}^\dagger \tilde{d}_{m\sigma} \tilde{d}_{m'\sigma'} : . \end{aligned} \quad (13)$$

The brackets  $:\hat{O}:$  indicate that the operator  $\hat{O}$  within the brackets must be normal ordered with respect to the ground state of the interacting system, which plays the role of the vacuum. This is because the interaction terms only come into play when more than one quasiparticle is created from the vacuum.

The renormalized Hamiltonian is not equivalent to the original model, and the relation between the original and renormalized model is best expressed in the Lagrangian formulation, where frequency enters explicitly<sup>11</sup>. For simplicity, we consider the case in the absence of a magnetic field, where the energy levels  $\epsilon_{dm\sigma}$  are independent of  $m$  and  $\sigma$ . If the Lagrangian density  $\mathcal{L}(\epsilon_d, \Delta, U, J_H)$  describes the original model, then by suitably re-arranging the terms we can write

$$\mathcal{L}(\epsilon_d, \Delta, U, J_H) = \mathcal{L}(\tilde{\epsilon}_d, \tilde{\Delta}, \tilde{U}, \tilde{J}_H) + \mathcal{L}_c(\lambda_1, \lambda_2, \lambda_3, \lambda_4), \quad (14)$$

where the remainder part  $\mathcal{L}_c(\lambda_1, \lambda_2, \lambda_3, \lambda_4)$  is known as the counter term and takes the form,

$$\begin{aligned} \mathcal{L}_c(\lambda_1, \lambda_2, \lambda_3, \lambda_4) = \sum_{m\sigma} \tilde{d}_{m\sigma}(\tau) (\lambda_2 \partial_\tau - \lambda_1) \tilde{d}_{m\sigma}(\tau) \\ + (\lambda_3 - \lambda_4) \sum_{mm'\sigma\sigma'} \tilde{d}_{m,\sigma}(\tau) \tilde{d}_{m'\sigma'}^\dagger(\tau) \tilde{d}_{m'\sigma'}(\tau) \tilde{d}_{m\sigma}(\tau) \\ + \lambda_4 \sum_{mm'\sigma\sigma'} \tilde{d}_{m\sigma}(\tau) \tilde{d}_{m'\sigma'}^\dagger(\tau) \tilde{d}_{m,\sigma'}(\tau) \tilde{d}_{m'\sigma}(\tau), \end{aligned} \quad (15)$$

where  $\lambda_1 = -\Sigma(0)$ ,  $\lambda_2 = z - 1$ ,  $\lambda_3 = (z^2 U - \tilde{U})/2$  and  $\lambda_4 = (\tilde{J}_H - z^2 J_H)/2$ . Though we can express the coefficients  $\lambda_i$ ,  $i = 1, 2, 3, 4$ , explicitly in terms of the self-energy terms and vertices at zero frequency, these relations are not useful in carrying out the expansion. We want to work entirely with the renormalized parameters and carry out the expansion in powers of  $\tilde{U}$  and  $\tilde{J}_H$ . We

assume that the  $\lambda_i$  can be expressed in powers of  $\tilde{U}$  and  $\tilde{J}_H$ , and determine them order by order from the conditions that there should be no further renormalization of quantities taken to be already fully renormalized. These conditions are

$$\tilde{\Sigma}_{m\sigma}(0,0) = 0, \quad \left. \frac{\partial \tilde{\Sigma}_{m\sigma}(\omega,0)}{\partial i\omega} \right|_0 = 0, \quad (16)$$

and that the renormalized 4-vertex at zero frequency,  $\tilde{\Gamma}_{m_1\sigma_1;m_2\sigma_2;m_3\sigma_3;m_4\sigma_4}(0,0,0,0)$  is such that

$$\begin{aligned} & \tilde{\Gamma}_{m_1\sigma_1;m_2\sigma_2;m_3\sigma_3;m_4\sigma_4}(0,0,0,0) = \\ & (\tilde{U} - \tilde{J}_H)(\delta_{m_4}^{m_1}\delta_{m_3}^{m_2}\delta_{\sigma_4}^{\sigma_1}\delta_{\sigma_3}^{\sigma_2} - \delta_{m_3}^{m_1}\delta_{m_4}^{m_2}\delta_{\sigma_3}^{\sigma_1}\delta_{\sigma_4}^{\sigma_2}) \\ & + \tilde{J}_H(\delta_{m_3}^{m_1}\delta_{m_4}^{m_2}\delta_{\sigma_4}^{\sigma_1}\delta_{\sigma_3}^{\sigma_2} - \delta_{m_4}^{m_1}\delta_{m_3}^{m_2}\delta_{\sigma_3}^{\sigma_1}\delta_{\sigma_4}^{\sigma_2}). \end{aligned} \quad (17)$$

In the field theory context these conditions are more commonly known as the renormalization conditions. They follow directly from the definitions of the renormalized self-energy in Eq. (7) and the definitions of the renormalized parameters given in Eq. (10).

The propagator in the RPT is the free quasiparticle Green's function,

$$\tilde{G}_{d,m\sigma}^{(0)}(\omega_n) = \frac{1}{i\omega_n - \tilde{\epsilon}_{dm\sigma} + i\tilde{\Delta}\text{sgn}(\omega_n)} \quad (18)$$

The spectral density of the corresponding retarded Green's function gives the free quasiparticle density of states,  $\tilde{\rho}_{m\sigma}^{(0)}(\omega)$  given by

$$\tilde{\rho}_{m\sigma}^{(0)}(\omega) = \frac{\tilde{\Delta}/\pi}{(\omega - \tilde{\epsilon}_{dm\sigma})^2 + \tilde{\Delta}^2}. \quad (19)$$

From Fermi liquid theory, the quasiparticle interaction terms do not contribute to the linear specific heat coefficient  $\gamma$  of the electrons. It follows that the impurity contribution to this coefficient is proportional to the free quasiparticle density of states evaluated at the Fermi level and is given by

$$\gamma = \frac{\pi^2}{3} \sum_{m,\sigma} \tilde{\rho}_{m\sigma}^{(0)}(0). \quad (20)$$

In the absence of a magnetic field this reduces to  $\gamma = 2n\pi^2\tilde{\rho}^{(0)}(0)/3$ , where  $\tilde{\rho}^{(0)}(0)$  is the quasiparticle density of states per single spin and channel.

If we integrate the free quasiparticle density of states in Eq. (19) to the Fermi level then we get  $\langle \tilde{n}_{dm\sigma} \rangle$  at  $T = 0$ , which is given by

$$\langle \tilde{n}_{dm\sigma} \rangle = \frac{\eta_{m\sigma}}{\pi} = \frac{1}{2} - \frac{1}{\pi} \tan^{-1} \left( \frac{\tilde{\epsilon}_{dm\sigma}}{\tilde{\Delta}} \right), \quad (21)$$

which defines the phase shift  $\eta_{m\sigma}$  in the channel with quantum numbers  $m$  and  $\sigma$ . For this model it has been shown by Shiba<sup>16</sup> that  $\langle n_{dm\sigma} \rangle = \eta_{m\sigma}/\pi$ , giving a generalization of the Friedel sum rule, so that we have

$\langle \tilde{n}_{dm\sigma} \rangle = \langle n_{dm\sigma} \rangle$ ; the quasiparticle occupation number in each channel is equal to the impurity occupation number in that channel. However, Yoshimori and Zawadowski<sup>17</sup> have shown that this form of the Friedel sum rule does not hold for a more general model in which scattering processes can occur between  $m$ -states,  $m_1, m_2 \rightarrow m_3, m_4$ , such that  $m_1 + m_2 = m_3 + m_4$ . They derive a restricted form of the sum rule such that  $\sum_{m\sigma} a_{m\sigma} \langle \tilde{n}_{dm\sigma} \rangle = \sum_{m\sigma} a_{m\sigma} \eta_{dm\sigma}/\pi$ , where  $a_{m\sigma} = 1, \sigma, m$ . In this more general case, therefore, the quasiparticle number does not equal the occupation number in the same channel but we have the more restricted result,  $\sum_{m\sigma} a_{m\sigma} \langle \tilde{n}_{dm\sigma} \rangle = \sum_{m\sigma} a_{m\sigma} \langle n_{dm\sigma} \rangle$ . Using either result, however, we can derive expressions for the zero field spin  $\chi_s$ , orbital  $\chi_{orb}$  and charge  $\chi_c$  susceptibilities. We differentiate the combinations,  $\sum_{m\sigma} a_{m\sigma} \langle \tilde{n}_{d,m\sigma} \rangle$ , with  $a_{m\sigma} = \sigma, m$  and 1 respectively, with respect to the magnetic field or in the charge case with respect to  $\tilde{\epsilon}_d$ . To evaluate these expressions we need to calculate the renormalized self-energy. This calculation taken to first order in  $\tilde{U}$  and  $\tilde{J}_H$  proceeds as in the one channel case<sup>10,11</sup>, and gives

$$\chi_s = 2n\mu_B^2 \tilde{\rho}^{(0)}(0)(1 + (\tilde{U} + (n-1)\tilde{J}_H)\tilde{\rho}^{(0)}(0)), \quad (22)$$

$$\chi_{orb} = \frac{(n^2 - 1)\mu_B^2 \tilde{\rho}^{(0)}(0)}{12} \left( 1 + (\tilde{U} - 3\tilde{J}_H)\tilde{\rho}^{(0)}(0) \right), \quad (23)$$

and

$$\chi_c = 2n\tilde{\rho}^{(0)}(0)(1 - ((2n-1)\tilde{U} - 3(n-1)\tilde{J}_H)\tilde{\rho}^{(0)}(0)). \quad (24)$$

These results can also be obtained from a mean field theory on the quasiparticle part of the Hamiltonian given in Eq. (13)<sup>18,19</sup>. It can be shown using the Ward identities derived by Yoshimori<sup>15</sup>, which are generalizations of the Ward identities derived by Yamada<sup>20,21</sup> for the single channel case, that these results are exact. Hence all higher order correction terms in  $\tilde{U}$  and  $\tilde{J}_H$  cancel out.

In the localized regime a large value of  $U$  suppresses the charge fluctuations on the impurity so  $\chi_c \sim 0$ . Treating this as an equality, we get a relation between  $\tilde{\rho}^{(0)}(0)$ ,  $\tilde{U}$  and  $\tilde{J}_H$ ,

$$((2n-1)\tilde{U} - 3(n-1)\tilde{J}_H)\tilde{\rho}^{(0)}(0) = 1. \quad (25)$$

When  $J_H = 0$ , this reduces to

$$\tilde{U}\tilde{\rho}^{(0)}(0) = \frac{1}{(2n-1)}, \quad (26)$$

For the case of half-filling, where  $\tilde{\epsilon}_d = 0$  and  $\tilde{\rho}^{(0)}(0) = 1/\pi\tilde{\Delta}$ , the non-linear relation between the renormalized parameters in Eq. (25) becomes a linear relation between  $\tilde{\Delta}$ ,  $\tilde{U}$  and  $\tilde{J}_H$ ,

$$\pi\tilde{\Delta} = (2n-1)\tilde{U} - 3(n-1)\tilde{J}_H. \quad (27)$$

For  $J_H = 0$  we get

$$\tilde{U} = \frac{\pi\tilde{\Delta}}{(2n-1)}, \quad (28)$$

which agrees with the one channel result  $\tilde{U} = \pi\tilde{\Delta}$  for  $n = 1$ .

When  $J_H = 0$  and we are in the localized limit, we have only one energy scale which we can take to be the Kondo temperature, defined for general  $n$  such that  $\gamma = \pi^2 n / 6T_K$ , equivalent to taking  $\tilde{\rho}^{(0)}(0) = 1/4T_K$ . In this limit the result for the Wilson ratio,  $R_W = \pi^2 \chi_s / 3\mu_B^2 \gamma = 2n/(2n-1)$ . This is the same as that for the  $N$ -fold degenerate Anderson model used to describe rare earth impurities for  $N = 2n$ . This result could have been anticipated, because the models can be shown to be equivalent by putting the orbital  $m$  and spin indices  $\sigma$  into a combined index  $\nu = (m, \sigma)$ <sup>22</sup>.

Switching on the interaction  $J_H (> 0)$  will reduce the local orbital fluctuations, as the configuration with the spins aligned will be favored. For  $J_H \gg \pi\Delta$  we can expect the orbital fluctuations to be almost fully suppressed so that  $\chi_{orb} \sim 0$  which, as an equality, gives a further relation between  $\tilde{\rho}^{(0)}(0)$ ,  $\tilde{U}$  and  $\tilde{J}_H$ ,

$$(3\tilde{J}_H - \tilde{U})\tilde{\rho}^{(0)}(0) = 1. \quad (29)$$

At half-filling this gives another linear relation between  $\tilde{\Delta}$ ,  $\tilde{U}$  and  $\tilde{J}_H$ ,

$$\pi\tilde{\Delta} = 3\tilde{J}_H - \tilde{U}. \quad (30)$$

An equivalent condition to that in Eq. (30) can be obtained using the argument of Nozières and Blandin<sup>23</sup> that the occupation number in a channel  $m$  should be independent of any small change in the chemical potential in a channel  $m' \neq m$  in this regime. When both the local charge and orbital fluctuations are suppressed, the renormalized parameters can be expressed in terms of the Kondo temperature  $T_K$ . From Eq. (25) and (29) we deduce

$$\tilde{U} = \frac{3}{2}\tilde{J}_H = 4T_K. \quad (31)$$

for the particle-hole symmetric case we have  $1/\tilde{\rho}^{(0)}(0) = \pi\tilde{\Delta} = 4T_K$ , so then we have

$$\pi\tilde{\Delta} = \tilde{U} = \frac{3}{2}\tilde{J}_H = 4T_K. \quad (32)$$

which was conjectured earlier on the basis of a phenomenological mean field approach<sup>18,19</sup>. A notable feature of this result is that there is no explicit dependence on  $n$ . In this regime from Eq. (22) we have for the spin susceptibility,

$$\chi_s = \frac{(g\mu_B)^2 S(S+1)}{3T_K}, \quad (33)$$

where  $S = n/2$  and  $g = 2$ , which leads to a Wilson ratio,  $R_W = 2(n+2)/3$ <sup>15,23</sup>.

Yoshimori<sup>15</sup> has also derived an exact result for the low temperature impurity contribution to the resistivity in the particle-hole symmetric case and  $H = 0$ . In terms of the renormalized parameters, the result is

$$R(T) = R_0 \left( 1 - \frac{\pi^4(1+2I_R)T^2}{3} + O(T^4) \right), \quad (34)$$

where  $I_R$  is given by

$$I_R = (\tilde{\rho}^{(0)}(0))^2 ((2n-1)\tilde{U}^2 - 6(n-1)\tilde{J}_H(\tilde{U} - \tilde{J}_H)). \quad (35)$$

This result can be derived in the RPT from a calculation of the renormalized self-energy  $\tilde{\Sigma}(\omega)$  to second order in  $\tilde{U}$  and  $\tilde{J}_H$ . With the Hund's rule interaction term, there are several types of second order scattering diagrams which are illustrated in Fig. 2. The vertices are of the same type as shown in Fig. 1 but are weighted by the renormalized interaction terms. The calculations follow along similar lines to those for the single channel case  $n = 1$ <sup>10,11</sup>. The first order diagrams and the terms linear in  $\omega$  are canceled by the counter terms to this order, and there are no corrections from the counter terms to the vertices to second order for the case with particle-hole symmetry. The contributions to  $I_R$  from diagrams of the types (i) to (iv) respectively in units of  $(\tilde{\rho}^{(0)}(0))^2$  are:  $\tilde{U}^2$ ;  $2(n-1)\tilde{J}_H^2$ ;  $2(n-1)(\tilde{U} - \tilde{J}_H)^2$ ;  $-2(n-1)\tilde{J}_H(\tilde{U} - \tilde{J}_H)$ ; which give the result in Eq. (35).

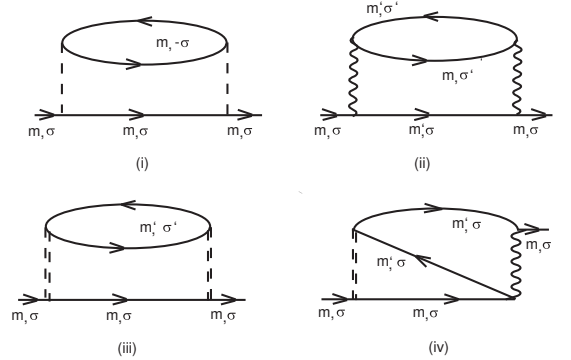


FIG. 2: (Color online) Second order diagrams in the renormalized perturbation theory.

In the localized regime at half-filling the result in Eq. (34) simplifies to give

$$R(T) = R_0 \left( 1 - \frac{\pi^4(5+4n)}{96} \left( \frac{T}{T_K} \right)^2 + O(T^4) \right), \quad (36)$$

which agrees with the result derived by Nozières<sup>24</sup> and Yamada<sup>20,21</sup> for the case  $n = 1$ . Thus all the exact Fermi liquid relations can be derived from the RPT taken to second order only.

It was shown in earlier work<sup>25</sup> that the RPT approach can provide a description of the dynamic spin susceptibility for the  $n = 1$  model in the low frequency regime. The

calculation takes account of the repeated quasiparticle scattering, giving results which are exact in the low frequency limit  $\omega \rightarrow 0$ , and in remarkably good agreement with the results from a direct NRG calculation. We extend the calculation to the  $n$ -channel model given in Eq. (1) and (2). We consider the Fourier transform of the transverse spin susceptibility,

$$\chi_s^{+-}(i\omega_{n'}) = \int_0^\beta \langle T_\tau \sum_m S_{d,m}^+(\tau) \sum_{m'} S_{d,m'}^-(0) \rangle e^{i\omega_{n'}\tau} d\tau, \quad (37)$$

where  $\omega_{n'} = 2\pi n'/\beta$  and  $S_{d,m}^+ = d_{m\uparrow}^\dagger d_{m\downarrow}$ ,  $S_{d,m}^- = d_{m\downarrow}^\dagger d_{m\uparrow}$  ( $S_{d,m}^z = (n_{d,\uparrow} - n_{d,\downarrow})/2$ ). We consider the scattering of a spin up quasiparticle with a spin down quasihole both in channel  $m$ , in the absence of a magnetic field. This particle-hole pair can scatter into a particle-hole pair in the same channel  $m$  or a different channel  $m' \neq m$ . We consider the scattering into the same channel first of all. The matrix element for this process is  $\tilde{U}$ , except we must allow for the fact that  $\tilde{U}$  already takes into account these processes for  $\omega = 0$  so, to prevent over-counting, we must use  $\tilde{U} - \lambda_3$ , where  $\lambda_3$  is the corresponding counter term. It will be convenient to use the notation  $\bar{U}$  for  $\tilde{U} - \lambda_3$ . Just taking this type of repeated scattering into account gives us a result which has the same form as in the single channel case  $n = 1$ <sup>25</sup>,

$$\chi_s^{+-}(\omega + i\delta) = 4n\mu_B^2 \frac{\tilde{\Pi}^{+-}(\omega + i\delta)}{1 - \bar{U}\tilde{\Pi}^{+-}(\omega + i\delta)}, \quad (38)$$

where we have analytically continued to real frequency  $\omega$ . The free quasiparticle-quasihole propagator in a single channel,  $\tilde{\Pi}^{+-}(\omega + i\delta)$ , is independent of the channel index in the absence of a magnetic field, and is given by

$$\begin{aligned} \tilde{\Pi}^{+-}(\omega + i\delta) &= \frac{\tilde{\Delta}}{\pi(\tilde{\epsilon}_d^2 + \tilde{\Delta}^2)}, \quad \omega = 0 \\ &= \frac{\tilde{\Delta}}{\pi\omega(\omega + 2i\tilde{\Delta})} \left\{ \ln \left( 1 + \frac{\omega}{\tilde{\epsilon}_d + i\tilde{\Delta}} \right) \right. \\ &\quad \left. + \ln \left( 1 - \frac{\omega}{\tilde{\epsilon}_d - i\tilde{\Delta}} \right) \right\} \quad \omega \neq 0, \end{aligned} \quad (39)$$

for  $\delta \rightarrow +0$ . We must also take into account that the quasiparticle-quasihole pair being created in channel  $m$  can scatter into a different channel  $m'$ , and also be finally annihilated in a channel with  $m' \neq m$ . The matrix element for this type of scattering is  $\tilde{J}_H$ , corresponding to the diagram in Fig. 1 (ii), but again, to avoid over-counting, we replace it by  $\bar{J}_H$ . In the absence of a magnetic field, the quasiparticle-quasihole propagator is independent of the channel index  $m$ , so the summation over the states  $m'$  introduces a factor  $n - 1$ . The result of taking these scattering processes into account is that the pair propagator  $\tilde{\Pi}^{+-}(\omega + i\delta)$  in Eq. (38) is replaced by

$$\frac{\tilde{\Pi}^{+-}(\omega + i\delta)}{1 - \bar{J}_H(n - 1)\tilde{\Pi}^{+-}(\omega + i\delta)}, \quad (40)$$

which leads to the result,

$$\chi_s^{+-}(\omega + i\delta) = 4n\mu_B^2 \frac{\tilde{\Pi}^{+-}(\omega + i\delta)}{1 - (\bar{U} + (n - 1)\bar{J}_H)\tilde{\Pi}^{+-}(\omega + i\delta)}. \quad (41)$$

We need to determine the combination  $\bar{U} + (n - 1)\bar{J}_H$ . We can do this by requiring that this expression gives  $2\chi_s$  in the zero frequency limit, which is equivalent to the requirement that these scattering processes contribute to the four vertex at zero frequency are not over-counted. This condition gives

$$\bar{U} + (n - 1)\bar{J}_H = \frac{\tilde{U} + (n - 1)\tilde{J}_H}{1 + (\tilde{U} + (n - 1)\tilde{J}_H)\tilde{\rho}^{(0)}(0)}. \quad (42)$$

In the Kondo regime this condition simplifies to  $\bar{U} + (n - 1)\bar{J}_H = 2T_K(1 + 2n)/(2 + n)$ , which gives the one channel result  $\bar{U} = 2T_K$  for  $n = 1$ .

By rewriting Eq. (41) in the form,

$$\frac{4n\mu_B^2}{\chi_s^{+-}(\omega + i\delta)} = \frac{1}{\tilde{\Pi}^{+-}(\omega + i\delta)} - (\bar{U} + (n - 1)\bar{J}_H), \quad (43)$$

and taking the imaginary part, it is straight forward to show that the expression for  $\chi_s(\omega)$  satisfies the exact Korringa-Shiba relation,

$$\lim_{\omega \rightarrow 0} \frac{\text{Im}\chi_s^{+-}(\omega + i\delta)}{\omega} = \frac{\pi\chi_s^2}{n\mu_B^2}, \quad (44)$$

which was proved for this model by Shiba<sup>16</sup> and more generally by Yoshimori and Zawadowski<sup>17</sup>.

So far we have not discussed how one can calculate the renormalized parameters  $\tilde{\epsilon}_d$ ,  $\tilde{\Delta}$ ,  $\tilde{U}$  and  $\tilde{J}_H$ . In the Kondo regime these reduce to a single parameter  $T_K$ , so one possibility is to deduce its value from experiment by fitting the predictions to the measurements of a physical quantity in the low temperature regime, say the impurity susceptibility or resistivity. Outside the Kondo regime we have four parameters to determine, and to calculate all four from experiment one loses much of the predictive power of the approach. However, it was shown earlier for the single channel Anderson model how the parameters,  $\tilde{\epsilon}_d$ ,  $\tilde{\Delta}$  and  $\tilde{U}$ , can be calculated in terms of the bare parameters,  $\epsilon_d$ ,  $\Delta$  and  $U$ , from the many-body low energy excitations of an NRG calculation<sup>12</sup>. There are problems in carrying out this procedure for the general  $n$ -channel model, due to the truncation of states which has to be carried out in an NRG calculation to reach the very low energy scales. Truncation means that only a fraction  $1/4^n$  states can be retained at each NRG iteration. It is possible, however, for the case  $n = 2$  to compensate for the lower percentage by increasing the number of states kept at each iteration as the matrices do not get so large. In the next section we present for calculations of  $\tilde{\Delta}$ ,  $\tilde{U}$ , and  $\tilde{J}_H$ , in terms of  $\Delta$ ,  $U$ , and  $J_H$ , for the  $n = 2$  model.

### III. NRG CALCULATION OF THE RENORMALIZED PARAMETERS FOR $N=2$

The two-channel model the Hamiltonian  $\mathcal{H}_d$  given in Eq. (2) can be re-expressed in the form,

$$\mathcal{H}_d = U \sum_{\alpha=1,2} n_{d\alpha\uparrow} n_{d\alpha\downarrow} + U_{12} \sum_{\sigma\sigma'} n_{d,1\sigma} n_{d,2\sigma'} - 2J_H \mathbf{S}_{d,1} \cdot \mathbf{S}_{d,2}, \quad (45)$$

with a ferromagnetic Heisenberg exchange coupling  $2J_H$  between the electrons in the different channels, and  $U_{12} = U - 3J_H/2$ . Our calculations will be restricted to the particle-hole symmetric model so we take  $\epsilon_d = -U/2 - U_{12}$  in the one-electron part of the Hamiltonian given in Eq. (1). The energy of the two electron triplet state of the isolated impurity with particle-hole symmetry is  $-2U + J_H$  and that of the 4-electron or 0-electron state is 0, so if we are interested in the case when the triplet state is the ground state configuration, we need to consider the regime  $U > J_H/2$ .

For the NRG calculations the model is recast in a form such that the impurity is coupled via a hybridization  $V$  to two tight binding chains which describe the conduction electron states, one chain for each channel. The conduction electron band is discretized with a discretization parameter  $\Lambda > 1$ , such that the couplings decrease along the chains as  $\Lambda^{-N/2}$  for large  $N$ , where  $N$  is the  $N$ th site along the chain from the impurity. The calculations are then carried out iteratively by direct diagonalization, starting at the impurity site and adding one further site to each chain at each iteration step. The number of basis states used has to be truncated when the matrices get too large for diagonalization on a practical timescale, which can occur after only a few iterative steps. When truncation is applied a fixed number of states is retained at each step. For the  $n=2$  model considered here, we take 3600 states, which is a factor of 3 to 4 more than for the non-degenerate model ( $n=1$ ) and a discretization factor  $\Lambda = 6$ . We can check the expected accuracy of our calculations by using this value for  $\Lambda$  to calculate  $\tilde{U}$  and  $\pi\tilde{\Delta}$  for the single channel model and compare with the values deduced indirectly from the exact Bethe ansatz results for the specific heat coefficient  $\gamma$  and the zero temperature spin susceptibility<sup>12</sup>. For  $U/\pi\Delta = 2$ ,  $\pi\Delta = 0.01$ , keeping 900 states, we get the values,  $\tilde{U} = 0.2295$  and  $\pi\tilde{\Delta} = 0.2387$ , which can be compared with those deduced from the Bethe ansatz,  $\tilde{U} = 0.2301$  and  $\pi\tilde{\Delta} = 0.2392$ . This gives an accuracy of better than 0.3%. For further details on setting up the NRG calculations, we refer to the original papers<sup>2,3</sup> and the recent review article<sup>26</sup>.

With this discrete spectrum the Green's function in Eq. (4) takes the form,

$$G_{d,\sigma}(\omega) = \frac{1}{i\omega - \epsilon_{dm\sigma} - |V|^2 g_{\alpha\sigma}(i\omega) - \Sigma_{m\sigma}(\omega)}, \quad (46)$$

where  $g_{\alpha\sigma}(i\omega)$  is the Green's function for the first site for the isolated conduction band chain.

The connection between the NRG approach and the renormalized perturbation theory is based on identifying the quasiparticle Hamiltonian, given in Eq. (12) and (13), as the low energy fixed point of the NRG together with the leading irrelevant terms<sup>27</sup>. The lowest single-particle excitations from the NRG ground state should correspond to a quasiparticle excitation described by the one-body part of the quasiparticle Hamiltonian as given in Eq. (12). For the calculation of the interaction terms,  $\tilde{U}$  and  $\tilde{J}_H$ , from the NRG we have to consider the difference between two-body excitations from the NRG ground state and the two corresponding one-body excitations.

The low energy single-particle excitations are given by the poles of the non-interacting quasiparticle Green's function when analytically continued to real frequency  $\omega$ . The equation for these poles is the same as that for the non-interacting model but with a renormalized hybridization  $\tilde{V}$  and energy level  $\tilde{\epsilon}_d$ . Therefore, the lowest energy single particle and hole excitations,  $E_p(N)$  and  $E_h(N)$ , from the *interacting* ground state should be solutions of the equation,

$$\omega - \tilde{\epsilon}_d - |\tilde{V}|^2 g_{\alpha\sigma}(\omega) = 0. \quad (47)$$

If we substitute the excitations energies,  $E_p(N)$  and  $E_h(N)$ , as calculated in the NRG for a finite chain length  $N$ , into Eq. (47) then we can deduce corresponding  $N$ -dependent renormalized parameters  $\tilde{V}(N)$  and  $\tilde{\epsilon}_d(N)$ . Only if  $\tilde{V}(N)$  and  $\tilde{\epsilon}_d(N)$  become independent of  $N$  for large  $N$ , do the low energy one-particle energy levels of the interacting system correspond to those of a renormalized non-interacting model. If this is the case, then the asymptotic values for large  $N$  define the renormalized parameters  $\tilde{V}$  (and hence  $\tilde{\Delta}$ ) and  $\tilde{\epsilon}_d$ .

To calculate the renormalized interaction terms, we first have to diagonalize the non-interacting impurity model with the renormalized parameters, which describes the quasiparticles. The interaction terms are then added to the quasiparticle Hamiltonian and expressed using the diagonalized single quasiparticle states as a basis. The energy difference between the lowest two-particle state and the sum of the corresponding two quasiparticle states is equal to the expectation value of interaction terms in the quasiparticle Hamiltonian. The interaction parameter  $\tilde{U}$  can be calculated from the NRG results for the lowest two-particle excitation in the *same* channel which will be independent of  $\tilde{J}_H$ . For a finite length chain  $N$  the value  $\tilde{U}(N)$  will depend upon  $N$ , and for this to correspond to a low energy quasiparticle Hamiltonian  $\tilde{U}(N)$  should become independent of  $N$  for large  $N$ . The asymptotic values of  $\tilde{U}(N)$  for large  $N$  defines the renormalized parameter  $\tilde{U}$ . Similarly, to calculate  $\tilde{J}_H$  we look at the difference between the single and triplet states of a two-particle excitation with one electron excitation in each of the two channels. This excitation will be independent of  $\tilde{U}$  and depend only on  $\tilde{J}_H$ . Using the NRG results for a finite chain of  $N$  sites, we can define a parameter  $\tilde{J}_H(N)$ , with  $\tilde{J}_H$  given by the asymptotic value



of  $\tilde{J}_H(N)$  for large  $N$ . Further details on the calculations of the renormalized parameters from the low energy NRG states can be found in reference<sup>12</sup>.

We first show results for the renormalized parameters as a function of  $N$ . We show a typical case in Fig. 3 for the parameters  $\tilde{U}(N)$ ,  $\pi\tilde{\Delta}(N)$  and  $3\tilde{J}_H(N)/2$  as a function of  $N$  for  $\pi\Delta = 0.01$ ,  $U/\pi\Delta = 3.6$  and  $J_H/\pi\Delta = 0.15$ , which is a parameter set corresponding to a point in the Kondo regime where the orbital fluctuations have been suppressed. The results demonstrate that not only is there a plateau region for all the parameters for large  $N$ , but also that the asymptotic values of  $\tilde{U}(N)$ ,  $\pi\tilde{\Delta}(N)$  and  $3\tilde{J}_H(N)/2$  correspond to a single energy scale and satisfy the relation given in Eq. (32). The choice of a relatively large value of  $\Lambda = 6$  means that the convergence to a plateau region is achieved for relatively small values of  $N$ . The plateau region is finite because the renormalized parameters correspond to the leading irrelevant corrections to the free fermion fixed point of the Wilson renormalization group transformation<sup>2</sup>, so eventually they diverge from the plateau when  $N$  is such that the decreasing irrelevant corrections become of the same order as the uncertainties in the numerical computation.

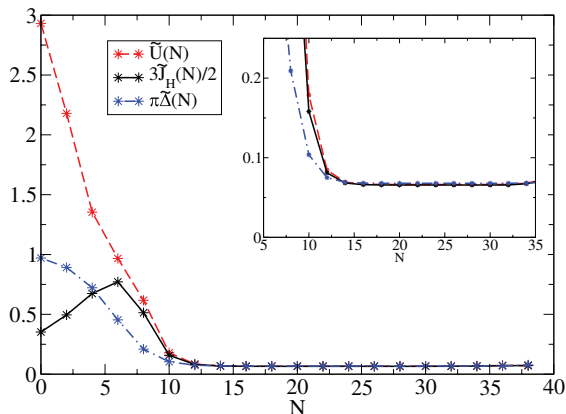


FIG. 3: (Color online) A plot of  $\tilde{\Delta}(N)/\pi\Delta$ ,  $\tilde{U}(N)/\pi\Delta$  and  $3\tilde{J}_H(N)/2\pi\Delta$  versus  $N$  for  $U/\pi\Delta = 3.6$ ,  $J_H/\pi\Delta = 0.15$  and  $\pi\Delta = 0.01$ . The inset shows the convergence of these parameter to a common limit in this case as the bare parameters correspond to a point in the Kondo regime.

We next look at the renormalized parameters in the different parameter regimes of the model. In Fig. 4 we show the results for  $\tilde{\Delta}/3\Delta$  and  $\tilde{U}/\pi\Delta$  versus  $U/\pi\Delta$  for  $J_H = 0$  ( $\pi\Delta = 0.01$ ). We predicted from Eq. (28) that for large  $U/\pi\Delta$  we should have a single energy scale such that for  $n = 2$ ,  $\tilde{U} = \pi\tilde{\Delta}/3$  and the results clearly show that this is the case for  $U/\pi\Delta > 3$ . The numerical results for the ratio  $\tilde{U}/\pi\tilde{\Delta}$  for large  $U$  give the value  $1/3$  to an

accuracy of 0.01%.

In Fig. 5 and 6 we compare the results for these two quantities with those for the single channel model  $n = 1$ . We can see that the parameters  $\tilde{\Delta}$  and  $\tilde{U}$  fall off with increase of  $U$  much more slowly for the two channel model. This is because in the two channel model we have unsuppressed fluctuations of the orbital component. When  $J_H = 0$  and finite  $U$ , at half-filling in the isolated impurity for the two channel model there are six degenerate two-electron configurations with energy  $2\epsilon_d + U$ . Both the  $n = 1$  and  $n = 2$  models in the Kondo regime can be described by localized  $SU(2n)$  Kondo model. For the case  $n = 1$  it is the s-d or  $SU(2)$  Kondo model and for  $n = 2$  the Coqblin-Schrieffer or  $SU(4)$  Kondo model. The Hamiltonian for the  $SU(2n)$  Kondo model takes the form,

$$\mathcal{H}_K(2n) = J_{\text{eff}} \sum_{\nu, \nu', k, k'} Y_{\nu, \nu'} c_{k', \nu'}^\dagger c_{k, \nu} + \sum_{\nu, k} \epsilon_k c_{k, \nu}^\dagger c_{k, \nu}, \quad (48)$$

where the sum over  $\nu = 1, 2, \dots, 2n$ , and with particle-hole symmetry  $J_{\text{eff}} = 4|V|^2/U$ . The operators  $Y_{\nu, \nu'}$  obey the  $SU(2n)$  commutation relations,

$$[Y_{\nu, \nu'}, Y_{\nu'', \nu'''}]_- = Y_{\nu, \nu'''} \delta_{\nu', \nu''} - Y_{\nu'', \nu'} \delta_{\nu, \nu'''}, \quad (49)$$

with  $\sum_{\nu} Y_{\nu, \nu} = nI$ . For  $n = 1$ ,  $Y_{\nu, \nu'} = |\nu\rangle\langle\nu'|$ , where  $|\nu\rangle$  are the single electron impurity states with spin up ( $\nu = 1$ ) and spin down ( $\nu = 2$ ), giving a two dimensional representation for the  $Y_{\nu, \nu'}$ . In the two channel case for half-filling the representation of the operators  $Y_{\nu, \nu'}$  is six dimensional and details of the  $Y_{\nu, \nu'}$  in terms of the two electron impurity states are given in the Appendix.

The relation  $T_K = \pi\tilde{\Delta}/4$  applies for both the  $n = 1$  and  $n = 2$  models in the case of particle-hole symmetry. In the single channel case  $n = 1$ ,  $T_K$  is known from the Bethe ansatz solution, and is given by  $T_K/\pi\Delta = \sqrt{u/2\pi} e^{-\pi^2 u/8 + 0.5/u}$ , where  $u = U/\pi\Delta$ <sup>28</sup>, and the NRG results for  $T_K$  deduced from  $\pi\tilde{\Delta}$  are in precise agreement with this expression for large  $U$ . For  $n \geq 2$  there is no Bethe ansatz solution for the model with finite  $U$ . However, there is a Bethe ansatz solution for the  $SU(N)$  Kondo model (Coqblin-Schrieffer model) and the  $N$ -fold degenerate Anderson model with  $U = \infty$ <sup>29–31</sup> which gives in the exponential for  $T_K$  a factor proportional to  $1/N$ . The prefactor is not universal and depends on the cut-offs used for the high energy excitations in the model. We have taken for the two channel case, therefore, the expression  $T_K/\pi\Delta = 1.01u e^{-\pi^2 u/16 + 0.25/u}/2\pi$ , where the prefactor has been chosen to give the most reasonable fit to the data. The result of this fitting is shown in Fig. 7, where it can be seen that the agreement is very good in the strong coupling range  $U/\pi\Delta > 4.0$ . The same form for  $T_K$  was used in reference<sup>22</sup>, and found to be in good agreement with their NRG results.



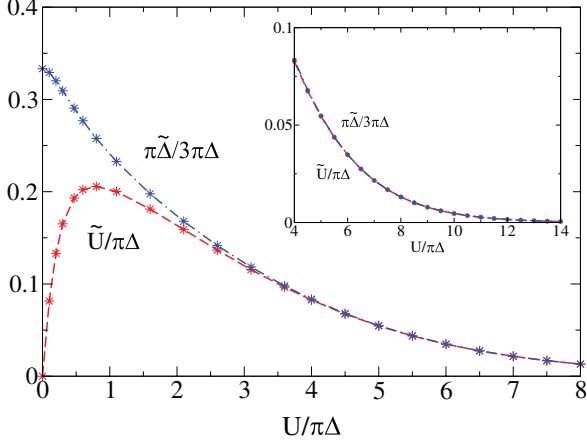


FIG. 4: (Color online) A plot of  $\tilde{\Delta}/3\pi\Delta$  and  $\tilde{U}/\pi\Delta$  versus  $U/\pi\Delta$  for  $J_H = 0$  and  $\pi\Delta = 0.01$ .

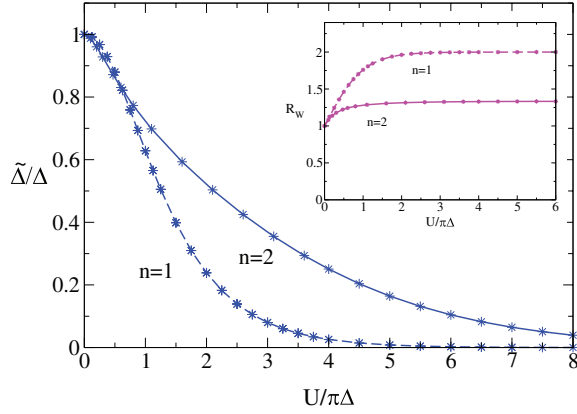


FIG. 5: (Color online) A comparison of  $\tilde{\Delta}/\Delta$  versus  $U/\pi\Delta$  for the  $n = 1$  and  $n = 2$  models for  $J_H = 0$  and  $\pi\Delta = 0.01$ . The inset shows the corresponding values for the Wilson ratio  $R_W = 1 + \tilde{U}/\pi\tilde{\Delta}$ .

In Fig. 8 we look at the effect of switching on the Hund's rule term  $J_H$  for a relatively large value of  $U$ ,  $U/\pi\Delta = 4.0$ , which is sufficient to suppress the charge fluctuations. As we increase  $J_H$ , we begin to suppress also the orbital fluctuations, such that when  $J_H/\pi\Delta > 0.1$  we are in the regime where we have a single energy scale. This we refer to as the Kondo regime with the Kondo temperature in the particle-hole symmetric case given by  $\pi\Delta = 4T_K$ . In

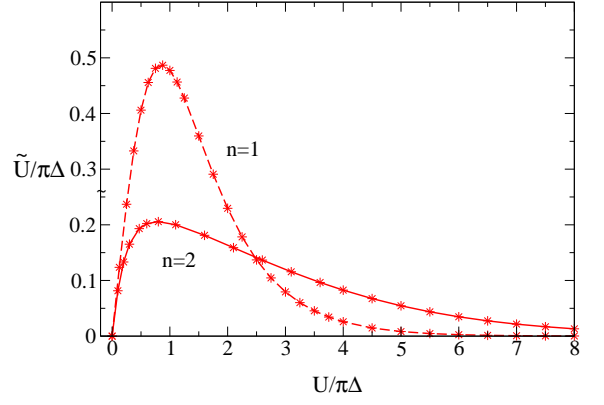


FIG. 6: (Color online) A comparison of  $\tilde{U}/\pi\Delta$  versus  $U/\pi\Delta$  for the  $n = 1$  and  $n = 2$  models for  $J_H = 0$  and  $\pi\Delta = 0.01$

this regime the relations between the renormalized parameters are such that  $\tilde{U}_{12} = \tilde{U} - 3\tilde{J}_H/2 = 0$ .

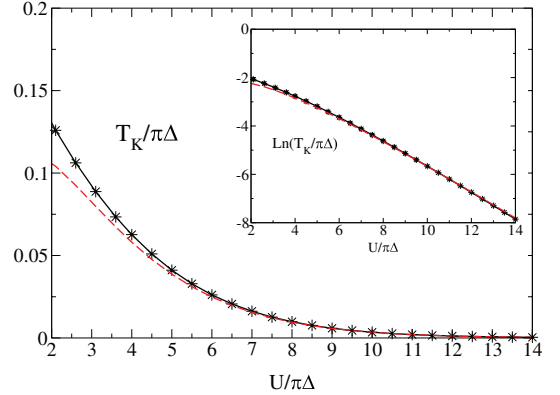


FIG. 7: (Color online) A plot of  $T_K/\pi\Delta$  ( $\pi\tilde{\Delta} = 4T_K$ ) as a function of  $U/\pi\Delta$  for  $J_H = 0$  and  $\pi\Delta = 0.01$ . The dashed curve corresponds to the formula  $1.01ue^{-\pi^2 u/16+0.25/u}/2\pi$ , where  $u = U/\pi\Delta$ . The inset shows a plot of the logarithm for the same two curves.

In Fig. 9 we plot the corresponding spin, orbital and charge susceptibilities using the expression for these given in Eq. (22), (23) and (24) for the set of parameters used for Fig. 8. The fact that the charge susceptibility is almost zero, due to the large value of  $U$ ,  $U/\pi\Delta = 4.0$ , means that the renormalized parameters must satisfy Eq. (27). This provides some insight into why the value of  $\tilde{U}$  increases initially as  $J_H$  is switched on. For small  $J_H$  the change in  $\tilde{J}_H$  is almost linear whereas the change in  $\pi\tilde{\Delta}$  is relatively small. Therefore to satisfy Eq. (27)  $\tilde{U}$  must also increase almost linearly in this region. We can also see from Fig. 9 that the orbital susceptibility is small

(multiplied by a factor 10 in the figure), and decreases monotonically as  $J_H$  increases.

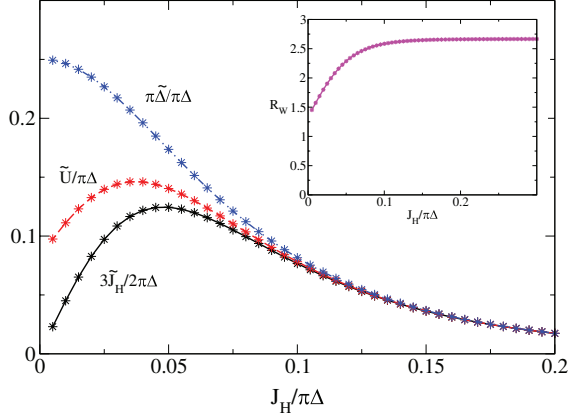


FIG. 8: (Color online) A plot of  $\pi\tilde{\Delta}/\pi\Delta$ ,  $\tilde{U}/\pi\Delta$ ,  $3\tilde{J}_H/2\pi\Delta$  versus  $J_H/\pi\Delta$  for  $U/\pi\Delta = 4.0$  and  $\Delta = 0.01$ . There is a single renormalized energy scale when  $J_H/\pi\Delta > 0.1$ . The inset shows the corresponding Wilson ratio  $R_W = 1 + (\tilde{U} + \tilde{J}_H)/\pi\tilde{\Delta}$ .

In Fig. 10 we explore a different parameter regime. Here the parameters  $\tilde{\Delta}$ ,  $\tilde{U}$ , and  $3\tilde{J}_H/2$  are plotted for a range of values of  $U$  for  $J_H/\pi\Delta = 0.05$ . We see that for this smaller value of  $J_H$  a large value of  $U/\pi\Delta \sim 5.5$  is required before the orbital fluctuations are suppressed and the Kondo regime is achieved. We suggest that the explanation for this behavior is that a large  $U$  strongly renormalizes the effective hopping parameter, which is proportional to  $\sqrt{\tilde{\Delta}}$ , so that the relatively weaker  $J_H$  is then sufficient to suppress the orbital fluctuations. The inset of Fig. 10 shows that the renormalized parameters do actually converge for  $U/\pi\Delta > 5.5$  to a common value. In Fig. 11 we plot the Wilson  $\chi_s/\gamma$  ratio,  $R_W = 1 + (\tilde{U} + \tilde{J}_H)/\pi\tilde{\Delta}$ , for the parameter set given in Fig. 10. It shows a steady increase from a value  $R_W \sim 1$  for small  $U$  with a leveling off at  $U/\pi\Delta \sim 5$  and then a convergence to the value  $R_W = 8/3$ , corresponding to that of the localized  $S = 1$  two channel Kondo model.

In the Kondo regime for the model with  $J_H \neq 0$  with particle-hole symmetry we have  $T_K = \pi\tilde{\Delta}/4$ . This regime occurs when  $J_H$  is large enough so that the triplet state of the impurity has a much lower energy than the other two-particle impurity states. The effective coupling of this state to the conduction electrons, via virtual transitions to either single particle or three particle impurity states induced by the hybridization, leads to an exchange

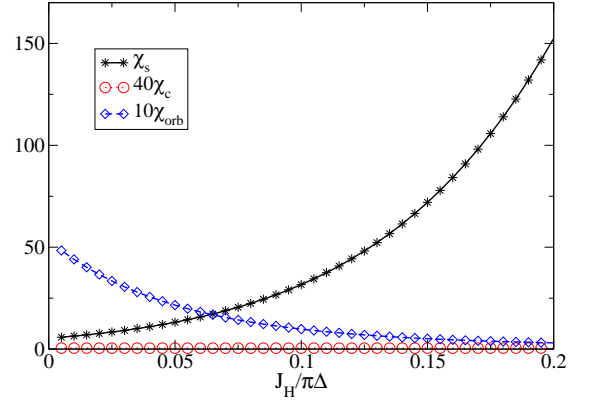


FIG. 9: (Color online) A plot of the spin susceptibility  $\chi_s$  (units of  $4\mu_B^2$ ),  $40 \times \chi_c$ , where  $\chi_c$  is the charge susceptibility, and the  $10 \times \chi_{orb}$ , where  $\chi_{orb}$  is the orbital susceptibility (units of  $\mu_B^2/4$ ), versus  $J_H/\pi\Delta$  for the same parameter set as in Fig. 8.

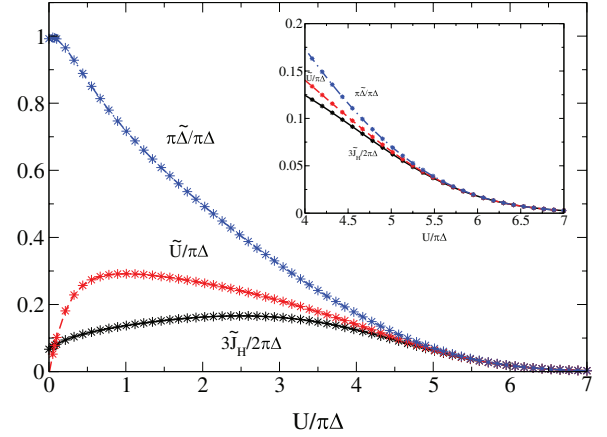


FIG. 10: (Color online) A plot of  $\pi\tilde{\Delta}/\pi\Delta$ ,  $\tilde{U}/\pi\Delta$  and  $3\tilde{J}_H/2\pi\Delta$  versus  $U/\pi\Delta$  for  $J_H/\pi\Delta = 0.05$  and  $\Delta = 0.01$ .

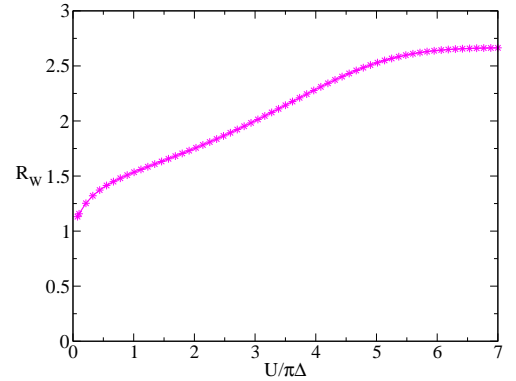


FIG. 11: (Color online) A plot of the Wilson ratio  $R_W = 1 + (\tilde{U} + \tilde{J}_H)/\pi\tilde{\Delta}$  versus  $U/\pi\Delta$  for  $J_H/\pi\Delta = 0.05$  and  $\Delta = 0.01$ .

model of a localized spin 1 coupled to the two channels of conduction electrons with an effective antiferromagnetic exchange interaction  $J_{\text{eff}} = 4V^2/(U + J_H)$ . This in turn will lead to a  $J_H$ -dependent term in the Kondo temperature of the form  $T_K \sim \exp(-a\pi^2 J_H/\pi\Delta)$ , where  $a$  is a dimensionless numerical coefficient. This implies that in the Kondo regime  $T_K$  will vary exponentially with  $J_H/\pi\Delta$ . In Fig. 12 we plot  $T_K$  from the NRG results against  $J_H/\pi\Delta$  and compare them with an exponential fit. The inset shows the plot of the logarithm of  $T_K$ ,  $\text{Ln}(T_K/\pi\Delta)$ , versus  $J_H/\pi\Delta$ . It can be seen that the exponential form does fit well with the results for the Kondo range  $J_H/\pi\Delta > 0.1$  with the value  $a = 1.49$ . There is a slight deviation for the largest values of  $J_H$  shown, but the coefficient  $a$  depends on the range chosen for the curve fitting.

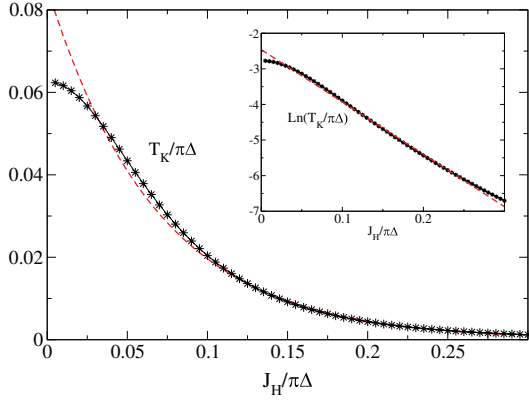


FIG. 12: (Color online) A plot  $T_K/\pi\Delta$  (full curve) and  $0.0854\exp(-1.49\pi^2 J_H/\pi\Delta)$  (dotted curve) versus  $J_H/\pi\Delta$  for  $U/\pi\Delta = 4$ ,  $\Delta = 0.01$ . The inset shows the  $\text{Ln}(T_K/\pi\Delta)$  and  $-1.49\pi^2 J_H/\pi\Delta + \text{Ln}(0.0854)$ .

Using the renormalized parameters for values of  $J_H/\pi\Delta = 0.05$  and  $J_H/\pi\Delta = 0.15$  taken from fig. 9 corresponding to  $U/\pi\Delta = 4$  and  $\Delta = 0.01$ , we have evaluated the expressions for the dynamic spin susceptibility given in Eq. (41). The result for the real part is shown in Fig. 13. It illustrates the narrowing and height increase of the central peak with the larger value of  $J_H$ . In Fig. 14 the imaginary part of  $\chi_s^{+-}(\omega)$  is shown. The marked increase in the change of the gradient through the origin for the larger value of  $J_H$ , can be explained as a consequence of the Korrington-Shiba relation given in Eq. (44).

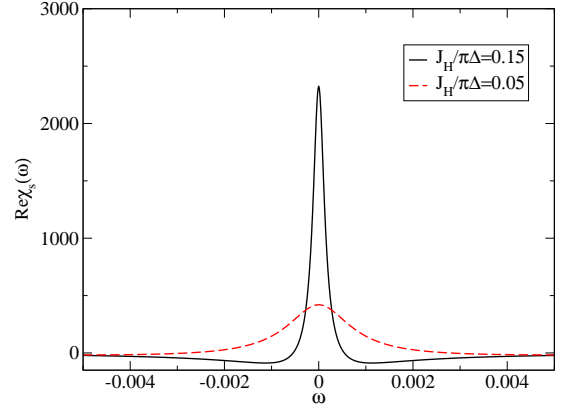


FIG. 13: (Color online) A plot of the real part of the dynamic spin susceptibility  $\chi_s^{+-}(\omega)$  (in units of  $8\mu_B^2$ ) for  $J_H/\pi\Delta = 0.05$  and  $J_H/\pi\Delta = 0.15$  with  $U/\pi\Delta = 4$ ,  $\Delta = 0.01$ .

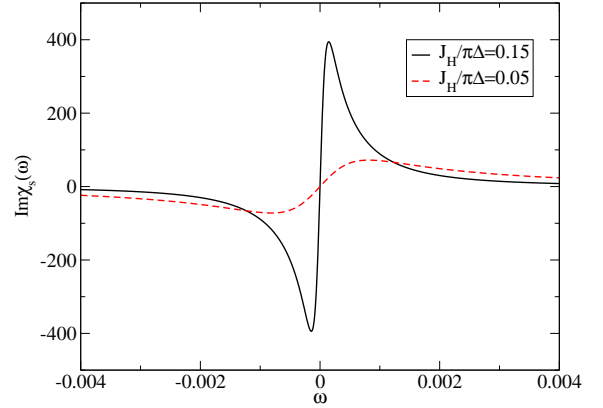


FIG. 14: (Color online) A plot of the imaginary part of the dynamic spin susceptibility  $\chi_s^{+-}(\omega)$  (in units of  $8\mu_B^2$ ) for  $J_H/\pi\Delta = 0.05$  and  $J_H/\pi\Delta = 0.15$  with  $U/\pi\Delta = 4$ ,  $\Delta = 0.01$ .

#### IV. CONCLUSIONS

The point of this study here for the  $n$ -channel Anderson model has been to show how the renormalized perturbation approach (RPT) can provide an asymptotically exact way of calculating the low temperature and low frequency behavior of the model in all parameter regimes. There have been many previous studies of related multi-orbital impurity models using a variety of approaches. The general  $n$ -channel Anderson model with finite  $U$  has not so far been solved using the Bethe ansatz, but there are exact solutions using this technique for the  $n$ -channel Kondo model coupled to a spin  $S^{29,30,32}$  and the  $n$ -channel Anderson model in the infinite  $U$  limit. In the latter case the impurity occupation number is restricted to the range  $n_d \leq 1^{31}$ . The main focus of the work on the  $n$ -channel Kondo model, however, has been on the over-screened case for  $n \geq 2S$ , where  $S$  is the spin of the impurity, as the model has a low energy non-Fermi

liquid fixed point. There have been many NRG studies of multi-orbital models and this work has been surveyed in the NRG review article<sup>26</sup>. The concern in most of the NRG work, however, has been with the calculation of the one-electron spectral densities, and mainly for the models without the Hund's rule term. There has also been a recent study for the  $J_H = 0$  model using the local moment approach, which includes NRG calculations for the case  $n = 2^{22}$ , and NRG studies of capacitively coupled quantum dots<sup>13</sup>.

The main feature of the RPT approach is that the calculations are carried out in terms of renormalized parameters which have a clear physical meaning in terms of the quasiparticles and their interactions. For the  $n$ -channel model they correspond to renormalizations of the parameters,  $\epsilon_d$ ,  $\Delta$ ,  $U$  and  $J_H$ , which specify the model. In the strong correlation or Kondo regime all these parameters can be determined explicitly in terms of a single low energy parameter, the Kondo temperature  $T_K$ . For the case  $n = 2$ , we have been able to deduce the renormalized parameters from the low lying excitations in an NRG calculation. The NRG results have confirmed the relations we derived between the renormalized parameters in the Kondo regime. As we have explicit expressions in Eq. (20), (22), (23) and (24) for the specific heat coefficient, spin, orbital and charge susceptibilities at zero temperature, these quantities were calculated simply by substituting the renormalized parameters into the relevant formulae. This procedure is very accurate and bypasses the usual NRG method which involves a subtraction procedure to isolate the impurity component. As there is a large parameter space to explore we have restricted the NRG calculations here to the particle-hole symmetric case. However, the RPT results are valid in all parameter regimes and the behavior of the model away from particle-hole symmetry will be the subject of a separate publication.

In setting up the RPT no approximation has been made, other than the assumption that the self-energy and its derivative are real and non-divergent at the Fermi level  $\omega = 0$ . This means that there is the possibility of extending the results to higher temperatures and frequencies. Some preliminary results have been achieved by including diagrams beyond second order<sup>11,33</sup> for the single channel model and this topic is currently being studied. The RPT in the Keldysh formalism can also be applied to non-equilibrium behavior and has been applied to the calculation of the non-linear corrections to the differential conductance for a quantum dot<sup>34,35</sup>, including an arbitrary magnetic field<sup>36</sup>.

The RPT approach is not restricted to impurity models, but the calculation of the renormalized parameters

for lattice models presents more of a problem as the NRG method cannot in general be applied. However, for infinite dimensional lattice models one can use the dynamical mean field theory (DMFT) to map the model into an effective impurity one, so the NRG method can then be used. This approach has been used to calculate renormalized parameters for the one-band Hubbard and Hubbard-Holstein models<sup>37,38</sup>. The work presented here opens up the possibility of extending this method to the two-band Hubbard model with a Hund's rule coupling. We have found that the Hund's rule term plays an important role in enhancing the magnetic response in the 2-fold degenerate model. It is known that the single band Hubbard model does not provide a basis for explaining the occurrence of ferromagnetism in 3d metals, as it predicts a ferromagnetic ground state only in a very restricted parameter regime, very close to half-filling and for a value of  $U$  much greater than the band width. It is likely that the inclusion of the Hund's rule coupling is essential to describe ferromagnetism in 3d materials.

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## Appendix

For the particle-hole symmetric model with  $n = 2$ , the model given in Eq. (48) can be derived by taking account to order  $|V|^2$  the effects of virtual excitations from the 2-electron to the local 1-electron and 3-electron impurity states. We denote the 1-electron basis states,  $|1 \uparrow\rangle$ ,  $|1 \downarrow\rangle$ ,  $|2 \uparrow\rangle$  and  $|2 \downarrow\rangle$ , by  $|\nu\rangle$  with  $\nu = 1, 2, 3, 4$  respectively. The 2-electron states we denote by  $|\nu, \nu'\rangle$ , with  $\nu \neq \nu'$  and  $|\nu', \nu\rangle$  represents the same state. This gives a six dimensional basis set. In terms of the Hubbard operators  $X_{(\nu, \nu'):(\nu'', \nu''')} = |\nu, \nu'\rangle\langle\nu'', \nu'''|$ , the  $Y_{\nu, \nu'}$  are given by

$$Y_{\nu, \nu'} = \sum_{\nu'' \neq \nu, \nu'' \neq \nu'} (-1)^\alpha X_{(\nu, \nu'):(\nu'', \nu'')}, \quad (50)$$

for  $\nu' \geq \nu$ , where  $\alpha = 1$  if  $\nu < \nu'' < \nu'$ , otherwise  $\alpha = 0$ . The  $Y_{\nu', \nu}$  for  $\nu' > \nu$  can be deduced from (50) using  $Y_{\nu', \nu} = (Y_{\nu, \nu'})^\dagger$ .

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